AD-A041 031   ARMY MOBILITY EQUIPMENT RESEARCH AND DEVELOPMENT COMM--ETC   F/G 7/4
                COMPUTER TECHNOLOGY IN MATERIALS ANALYSIS, PART I. METALS AND A--ETC(U)
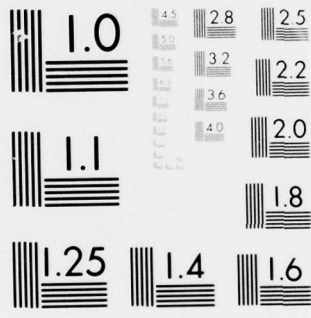   MAY 77   F L HARRIS
UNCLASSIFIED   MERADCOM-2210   NL

1 OF 1

AD
A041031

END
DATE
FILMED
7-77

MICROCOPY RESOLUTION TEST CHART
NATIONAL BUREAU OF STANDARDS-1963-A

ADA041031

AD

Report 2210

COMPUTER TECHNOLOGY IN MATERIALS ANALYSIS –

PART I, METALS AND ALLOYS

May 1977

U.S. ARMY MOBILITY EQUIPMENT

RESEARCH AND DEVELOPMENT COMMAND

FORT BELVOIR, VIRGINIA

REPORT DOCUMENTATION PAGE		READ INSTRUCTIONS BEFORE COMPLETING FORM
1. REPORT NUMBER 2210	2. GOVT ACCESSION NO.	3. RECIPIENT'S CATALOG NUMBER
4. TITLE (and Subtitle) COMPUTER TECHNOLOGY IN MATERIALS ANALYSIS, PART I. METALS AND ALLOYS		5. TYPE OF REPORT & PERIOD COVERED Interim rept.
		6. PERFORMING ORG. REPORT NUMBER
7. AUTHOR(s) F. L. Harris		8. CONTRACT OR GRANT NUMBER(s)
9. PERFORMING ORGANIZATION NAME AND ADDRESS Material Technology Laboratory U.S. Army Mobility Equipment Research and Development Command, Fort Belvoir, Virginia 22060		10. PROGRAM ELEMENT, PROJECT, TASK AREA & WORK UNIT NUMBERS PRON A1-3-P6350 AW-EF
11. CONTROLLING OFFICE NAME AND ADDRESS Army Materials and Mechanics Research Center ATTN: AMXMRA-QA Watertown, MA 02172		12. REPORT DATE May 1977
		13. NUMBER OF PAGES 22
14. MONITORING AGENCY NAME & ADDRESS(If different from Controlling Office)		15. SECURITY CLASS. (of this report) Unclassified
		15a. DECLASSIFICATION/DOWNGRADING SCHEDULE

16. DISTRIBUTION STATEMENT (of this Report)

Approved for public release; distribution unlimited.

17. DISTRIBUTION STATEMENT (of the abstract entered in Block 20, if different from Report)

MERADCOM - 2210

18. SUPPLEMENTARY NOTES

19. KEY WORDS (Continue on reverse side if necessary and identify by block number)

Spectrographic Analysis
Metals and Alloys
Computer-Aided Spectrographic Analysis

20. ABSTRACT (Continue on reverse side if necessary and identify by block number)

A system is described for computer processing of data obtained from photographed optical emission spectra of metals and alloys. Samples of computer-produced emulsion calibration curves and element concentration calibration curves are provided. A digital scanning densitometer acquired for more complete automation of the system is also discussed.
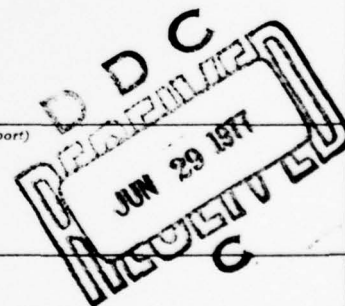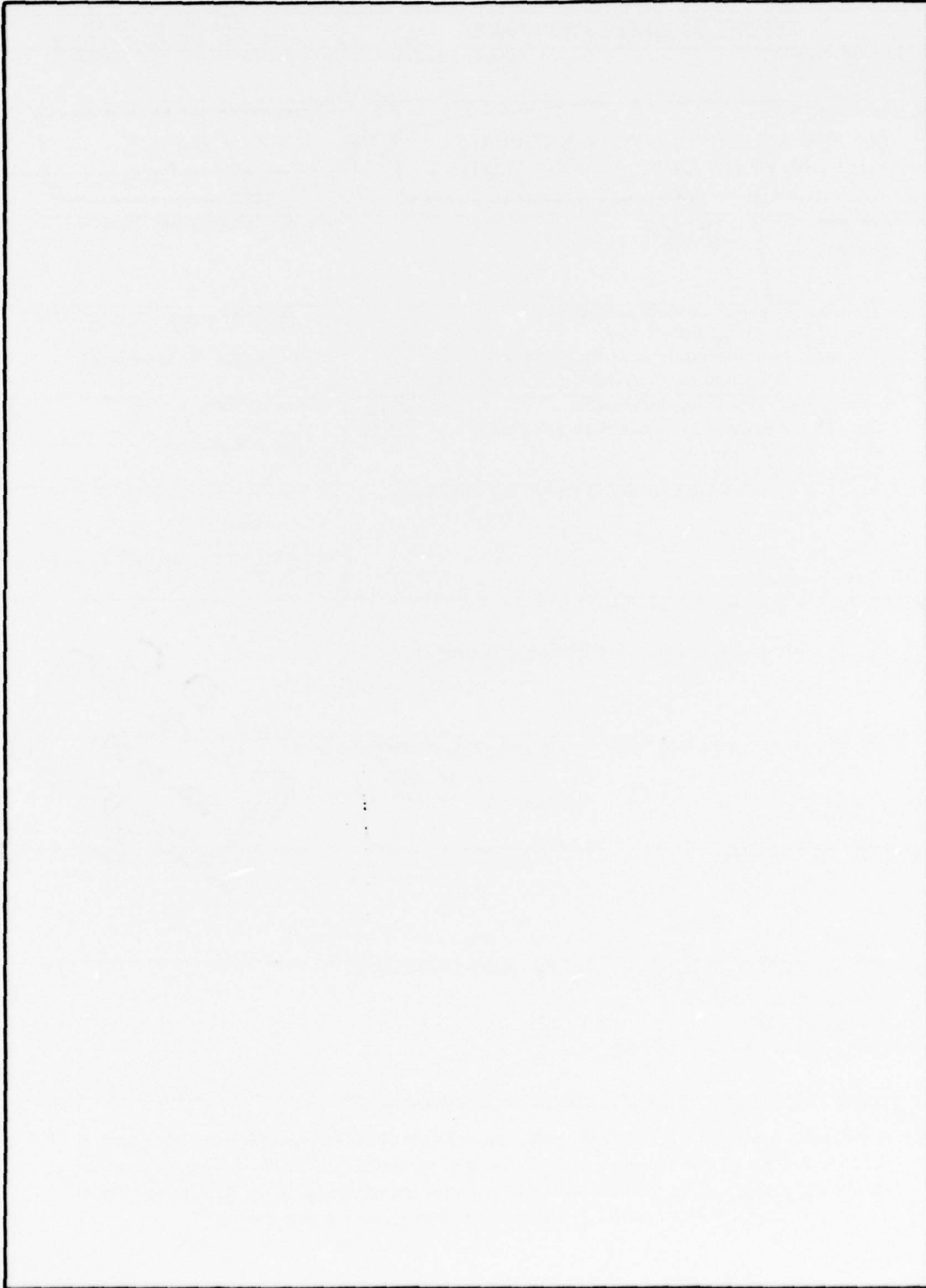
DD FORM 1473 EDITION OF 1 NOV 65 IS OBSOLETE

PREFACE

The work covered by this report was accomplished by Frank L. Harris under the direction of Emil J. York, Chief, Material Technology Laboratory, U.S. Army Mobility Equipment Research and Development Command. The effort constitutes a part of the U.S. Army Materials Testing Technology (MTT) program to provide better procedures in chemical, mechanical, and nondestructive testing techniques to increase inspection efficiency for material/materiel procured by the U.S. Army Materiel Development and Readiness Command. Technical contributions in program modification and conversion were made by Arthur L. Nickless, Scientific and Engineering Applications Division, Management Information Systems Office, MERADCOM.

iii

CONTENTS

COMPUTER TECHNOLOGY IN MATERIALS ANALYSIS –

PART I, METALS AND ALLOYS

I. INTRODUCTION

1. **Statement of the Problem.** To significantly decrease the time and effort required to evaluate photographed emission spectra used in the analysis of metals and alloys.

2. **Background.** Spectrographic techniques are used at MERADCOM for the analysis of many kinds of materials, ranging from ferrous and nonferrous metals to ceramics and paint pigments. This variety of sample types makes the use of rapid, direct-reading emission spectrographs impractical, and slower, photographic methods have been adopted. A faster means of obtaining quantitative answers from photographed emission spectra would constitute a significant advance in our materials testing and engineering capabilities.

At the present time, photographed spectra are evaluated by obtaining transmission values from a conventional microphotometer. The values for all spectral lines of interest are manually recorded on a printed form designed for this purpose. This is one of the most time-consuming and tedious portions of the analysis. To obtain transmission values for a completely filled plate, for example, can require several man-hours depending upon the number of spectral lines to be used in the analysis.

Still more time consuming is the treatment of the spectral line transmission values after they have been recorded. A slide rule type calculating device is used to construct a calibration curve for the photographic emulsion being used. This curve relates the percent transmission of a spectral line to the intensity of the light producing the line and is used to determine intensities for all lines used in the analysis. Finally, an analytical working curve is prepared by plotting line intensity against concentration using a set of known standard materials. A separate working curve is prepared for each element to be determined. Concentrations of unknown samples are then obtained by comparison of their line intensities to the working curve. The two avenues open for solution of the problem are: (1) increase the speed of acquiring transmission values, and (2) increase the speed of converting transmission values into concentrations. This report discusses the current status of the project and describes equipment acquired for the purpose of automatic acquisition of transmission values and how the MERADCOM computer is used to perform the tedious calculations and curve plotting required.

1

II. EXPERIMENTAL PROCEDURE

3.   Approach to the Problem. Several computer programs were obtained for the purpose of handling spectrographic data. The first of these, which is currently in routine use, requires that the transmission data be obtained from a conventional densitometer and entered into the computer on punched cards, along with the fixed data, such as the filter factor and the concentrations of the standards being used.

The computer then calculates all line intensities from the transmission data, plots the final emulsion calibration curve, plots all working curves, and computes answers for unknown samples. Figures 1 and 2 are examples of computer-plotted curves. Figure 1a is the final emulsion calibration curve for an SA No. 1 plate. Figure 1b gives the set of points used to plot the emulsion calibration curve of Figure 1a. Transmittances and corresponding intensities are given as well as the natural logarithms of these values. Figure 2a is a working curve for nickel in copper base alloys. Figure 2b gives the set of points used by the computer to plot the working curve of Figure 2a. The computer fits all of the above curves by a polynomial regression procedure and prints the regression coefficients of each curve.

A number of government and private laboratories have used computer technology to process transmission data taken from spectrographic plates with conventional densitometers. In recent years, however, digital scanning densitometers capable of acquiring transmission values rapidly and automatically have appeared on the market and computer programs have been developed to process transmission values obtained in this way. Such an instrument was recently acquired by this Laboratory (see Figure 3).

This instrument is designed to scan each spectrum on the plate with a beam of light which is sampled by a photomultiplier tube at a predetermined regular interval of scanned distance. The light sampling interval is selectable from five values ranging from 2.5 to 40 microns of travel along the plate and should be chosen to meet any constraints of spectrum line width as defined by a given computer program. Each time the phototube samples the light beam, it produces an analog electrical signal which is then digitized and recorded on magnetic tape. Approximately 100,000 readings are taken for each spectrum.

One of the several computer programs previously mentioned, developed at the US Geological Survey, is being modified to make its input routines compatible with our scanning densitometer. When modification is complete, much better accuracy will be attainable in reading tape-recorded spectra into the computer. The logic of this program enables it to find among the recorded transmission readings, spectrum lines whose wavelength, element symbol, estimated position along the plate, and other constants, have been read into the computer previously as fixed data, and then to calculate the

intensity of each line found, finally computing the concentration of each element sought.

4. **Results**. Although the system is not yet completely automated to do the actual plate reading, the computer is being used to perform the calculations and graphics required to obtain answers. This section presents a sample of results obtained for the analysis of a low alloy steel. The table compares results for the determination of silicon, nickel, and chromium using, in one case, the conventional manual calculating technique and, in the other, the computer.

Analysis of a Low Alloy Steel

Sample	Alloying Elements (%)					
	Silicon		Chromium		Nickel	
	Manual	Computer	Manual	Computer	Manual	Computer
Gear No. 1	0.31	0.34	0.49	0.49	0.47	0.51
Gear No. 2	0.31	0.29	0.43	0.48	0.46	0.47

III. DISCUSSION AND CONCLUSIONS

5. **Discussion**. The present status of the project allows the spectrographer to manually record transmission values on computer coding sheets in a format compatible with the program input statements. The coding sheets are then submitted to the computer center for keypunching. The punched data deck is read into the computer, relieving the spectrographer of the task of constructing emulsion calibration curves and working curves and of calculating results for unknowns. This represents a considerable saving in time; a low alloy steel, for example, can now be analyzed in half the time previously required with no loss in quantitative accuracy.

The table indicates that there is good agreement between the conventional manual technique and the computer for calculation of analytical results. As mentioned earlier, a third and final computer program, developed at the U.S. Geological Survey, is currently being modified to fit the requirements of the scanning densitometer shown in Figure 3. This program was originally written for use with a scanner which reads 20 inches of spectrum in one pass. At the present time, scanners with this capability are not available commercially. Most are designed to scan only 10 inches in a single pass. Modification of the program involves a rewriting of its input routines such that two 10-inch scans will appear to the computer as a single 20-inch pass. These modifications and the automated scanning system will be discussed in detail in a later report.
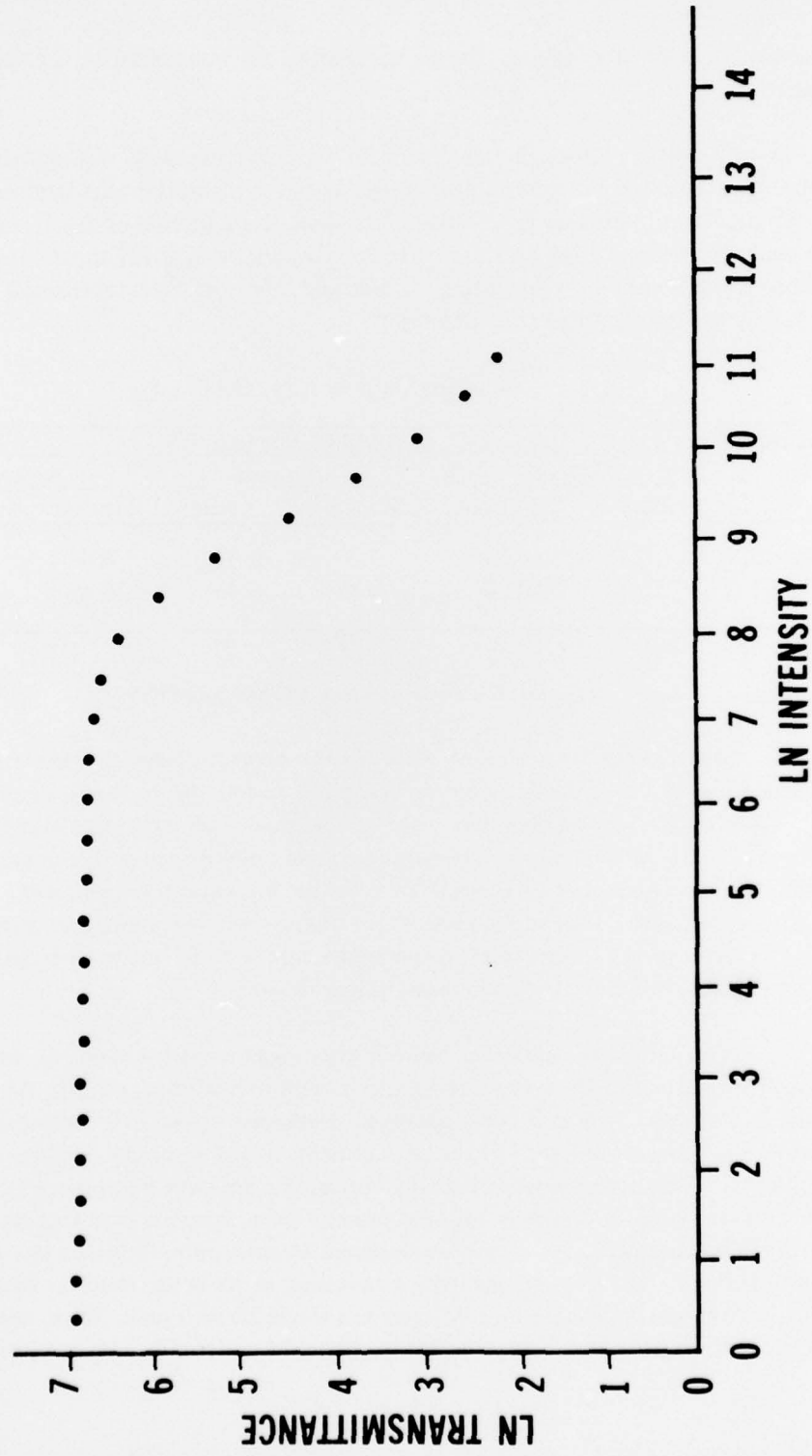
Figure 1a. Computer-plotted final emulsion calibration curve.

SET OF POINTS FOR FINAL PLATE CALIBRATION CURVE — PECC(1).

POINT NO.	LN INTENSITY	LN TRANSMITTANCE	NO.	INT	10x OT
1	.35167	6.90776	1	1	1000
2	.79635	6.90120	2	2	993
3	1.24104	6.89120	3	3	983
4	1.68572	6.88120	4	5	973
5	2.13041	6.87120	5	8	964
6	2.57510	6.86120	6	13	954
7	3.01978	6.85120	7	20	945
8	3.46447	6.84120	8	31	935
9	3.90915	6.83120	9	49	926
10	4.35384	6.82120	10	77	917
11	4.79853	6.81120	11	121	907
12	5.24321	6.80120	12	189	898
13	5.68790	6.79120	13	295	889
14	6.13258	6.78506	14	460	884
15	6.57727	6.76925	15	718	870
16	7.02195	6.72925	16	1120	836
17	7.46664	6.63201	17	1748	759
18	7.91133	6.41507	18	2728	610
19	8.35601	5.99989	19	4255	403
20	8.80070	5.35796	20	6638	212
21	9.24538	4.57013	21	10356	96
22	9.69007	3.78230	22	16156	43
23	10.13475	3.10988	23	25203	22
24	10.57944	2.59694	24	39318	13
25	11.02413	2.23416	25	61336	9

INFLEC. PT. AT   9.24538   4.57013

PLOTTING TAPE PREPARED.

Figure 1b. Set of points used to plot the emulsion calibration curve.

5

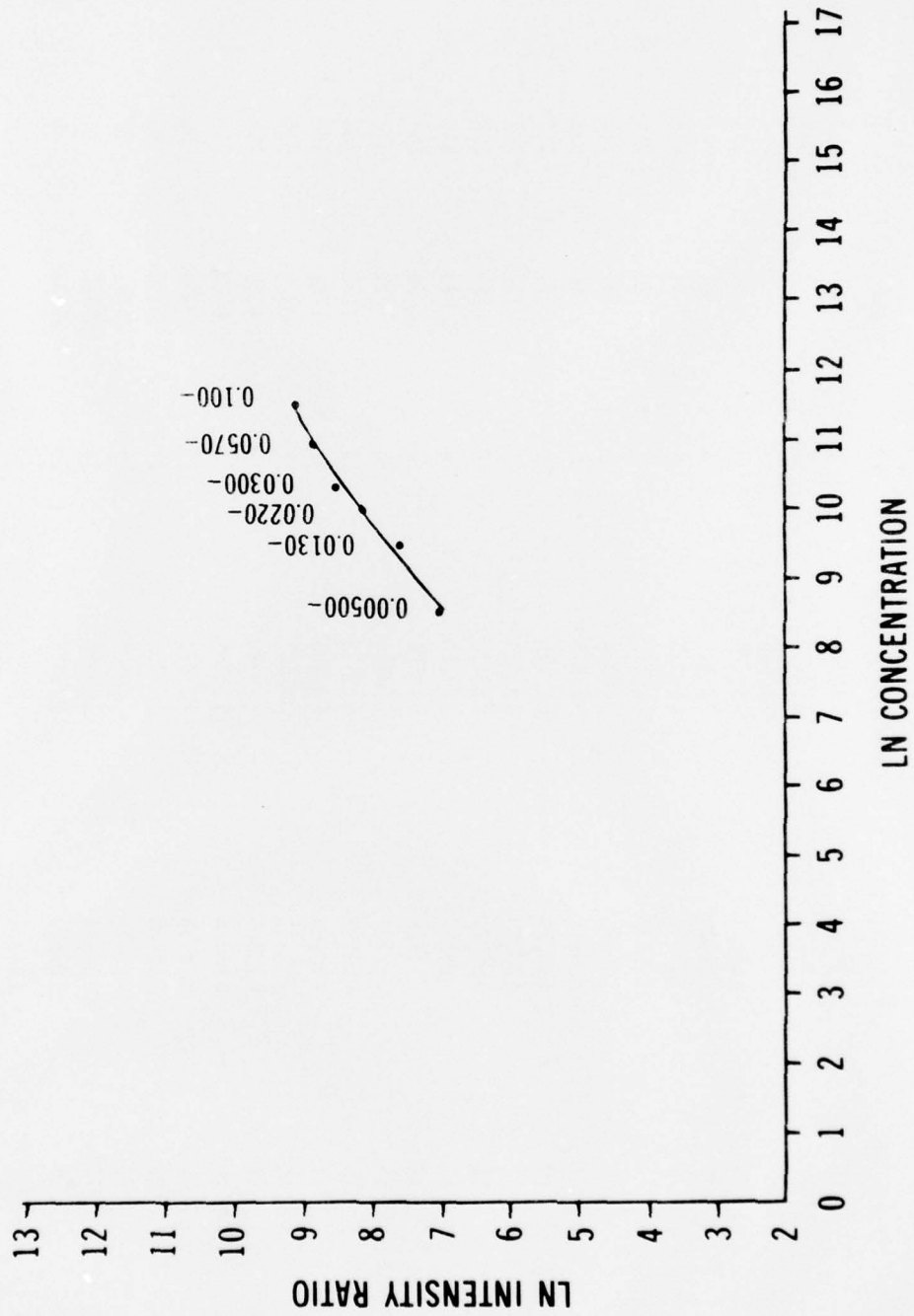# PERCENT NI IN COPPER W.O. 13672 5/22/75 NI 3414.760/BKGD

Figure 2a. Computer-plotted working curve for nickel in copper base alloys.

PERCENT NI IN COPPER W.O. 13672 5/22/75 NI 3414.760/BKGD

NO. 1-5

	TABLE OF RESIDUALS					TABLE OF EXPONENTIALS		
NO. POINT	X VALUE	Y VALUE	Y ESTIMATE	RESIDUAL	NO. POINT	X VALUE	Y VALUE	Y ESTIMATE
1	11.51293	9.09796	9.15418	.05622	1	100000	8937	9453
2	10.95081	8.85450	8.80797	.04652	2	57000	7005	6687
3	10.30895	8.50899	8.37602	.13297	3	30000	4959	4341
4	9.99880	8.12382	8.15329	-.02947	4	21999	3373	3474
5	9.47270	7.60875	7.75463	-.14588	5	12999	2015	2332
6	8.51719	7.01551	6.96344	.05208	6	4999	1113	1057

FORM OF EQUATION IS $Y = C + B(X) + A(X)(X)$ WHERE $Y = LN(INTENSITY)$
AND $X = LN(1,000,000 \text{ TIMES } 0 \text{ ELEMENT})$

COEF. - EQUA. NO. 1 A = SECOND DEGREE TERM...... -.04741718
B = FIRST DEGREE TERM....... 1.68105879
C = CONSTANT TERM.......... -3.91469906

STD. DEV. = .12632   VERTEX (X) = 17.72626

FOR PLOTTER

XARRAY	YARRAY	ZARRAY
8.51719	6.96344	7.01551
9.47270	7.75463	7.60875
9.99880	8.15329	8.12382
10.30895	8.37602	8.50899
10.95081	8.80797	8.85450
11.51293	9.15418	9.09796

SLOPE POINT(X) = 14.56285
POINTS POINT(Y) = 7.01550

USE AN UPPER LIMIT OF 11.51293   .589
USE A LOWER LIMIT OF   8.51719   .873

50 DEGREE SLOPE AT X = 5.07262
30 DEGREE SLOPE AT X = 11.39944

CLASS VALUE = 8.
96   4   0

0 VECTORS LOST
81 ACTIVE LINES USED
0 VECTORS LOST
81 ACTIVE LINES USED

PLOTTING TAPE PREPARED.

Figure 2b. Set of points used by the computer to plot the working curve for nickel in copper base alloys.

7

Figure 3. Digital scanning densitometer.

The calibration curves and numerical data appearing in the Appendix were generated by the computer during the analysis of the low alloy steel mentioned previously. The computer fits two curves for each element, one with concentration limits and one without; determines the regression coefficients for each; and suggests upper and lower concentration limits for each curve. All curves are fitted both as first-degree and second-degree polynomials, and the program classifies all of the second-degree curves on a scale of zero to ten based on a consideration of the following factors:

Class = 0 if less than three points are supplied.

Class = 1 for three points.

Class = 2 for four points if the standard deviation is greater than 0.5.

8

The class value may then range up to a maximum of 10 according to Walthall's formula:

Class Value = (Points factor + sigma factor + residual factor)/3 where:

Points factor = 4 if there are 4 points to fit, or
               = 10 for 5 or more points.
Sigma factor   = 6 if there are 4 points to fit, or
               = 1 if standard deviation is greater than 0.9, or
               = 10 – 10x standard deviation.
Residual factor = 10x (fraction of points having a residual less than or
                equal to 0.1).

The higher the class value, the more useful is the curve.

6. Conclusions.

a.   The computer programs described, although originally written for the analysis of silicate rocks, have been shown to be effective when applied to the analysis of metals and alloys, both ferrous and nonferrous.

b.   The two programs currently in use have completely eliminated the requirement for the calculating board for construction of calibration curves and the computation of concentrations.

c.   A third program to allow for the automated acquisition of transmission values from our scanning densitometer is currently undergoing modification to make it compatible with this equipment. It is expected that this last task will be completed in the near future.

REFERENCES

1.   A. W. Helz, F. G. Walthall, and Sol Berman, "Computer Analysis of Photographed Optical Emission Spectra." Applied Spectroscopy, 23, 5 (1969), p. 508.

2.   Frank G. Walthall, "Spectrochemical Computer Analysis." Program Description–Journal of Research, US Geological Survey 2.1 (1974), p. 61.

Working Curves and Numerical Output Used for the Analyses Reported in the Table, Page 3.

PERCENT SILICON IN LOW ALLOY STEEL SI 2881.6/BKGND
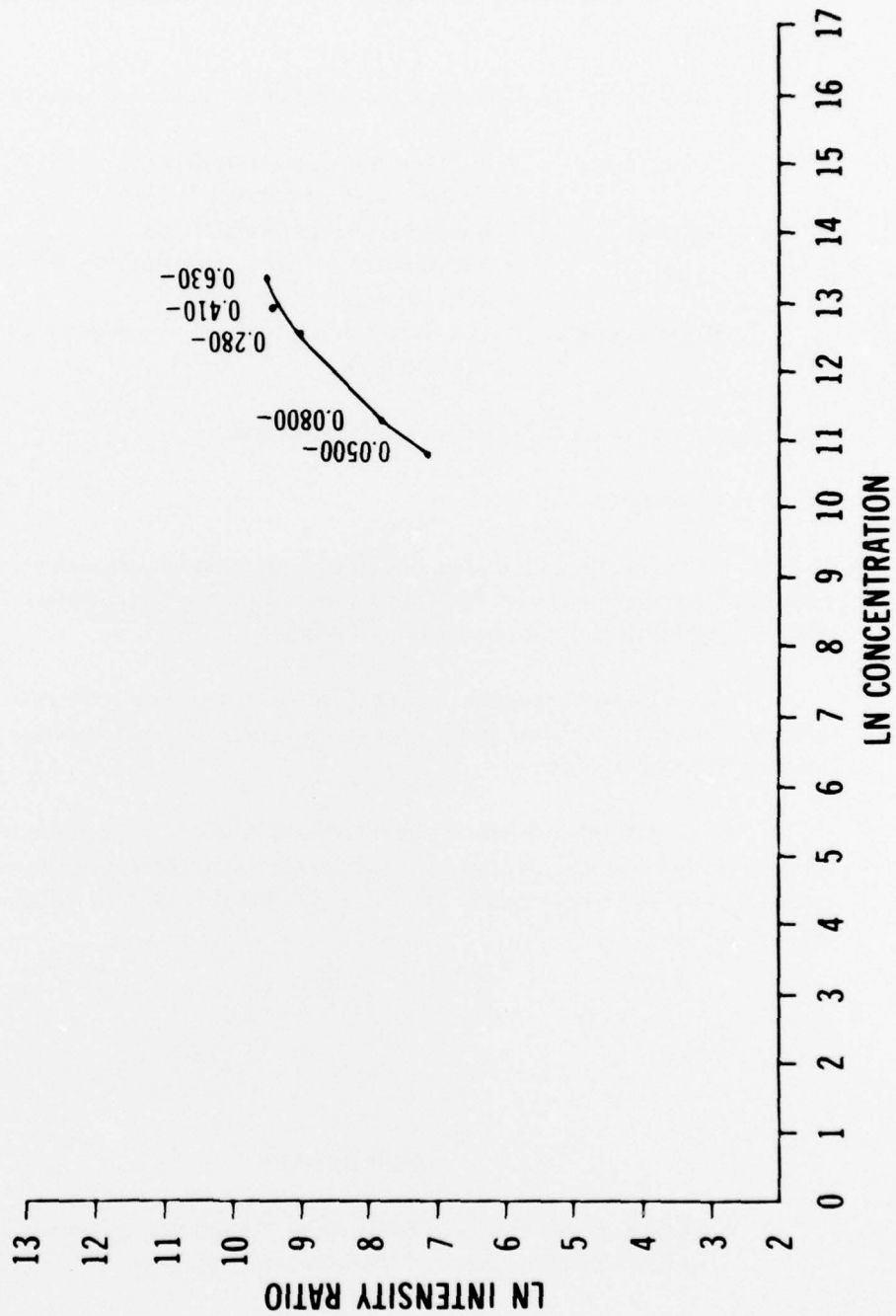
PERCENT SILICON IN LOW ALLOY STEEL SI 2881.6/BKGND

NO. 3-5

TABLE OF RESIDUALS

NO POINT	X VALUE	Y VALUE	Y ESTIMATE	RESIDUAL
1	13.35348	9.51258	9.54286	-.03029
2	12.92391	9.41566	9.32767	.08799
3	12.54254	9.00499	9.07179	-.06680
4	11.28978	7.81632	7.80210	.01423
5	10.81978	7.15088	7.15600	-.00512

TABLE OF EXPONENTIALS

NO. POINT	X VALUE	Y VALUE	Y ESTIMATE
1	629999	13528	13944
2	410000	12279	11244
3	280000	8143	8706
4	80000	2480	2445
5	50000	1275	1281

FORM OF EQUATION IS $Y = C + B(X) + A(X)(X)$ WHERE $Y = LN(INTENSITY)$
AND $X = LN(1,000,000$ TIMES 0 ELEMENT)

COEF. - EQUA. NO. 3   A = SECOND DEGREE TERM..... -.20963207
B = FIRST DEGREE TERM...... 6.00953666
C = CONSTANT TERM......... -33.32472850

STD. DEV. = .08170   VERTEX (X) = 14.33353

SLOPE POINT(X) = 13.61799
POINTS POINT(Y) = 7.15087

USE AN UPPER LIMIT OF 13.35348   .411
USE A LOWER LIMIT OF 10.81978   1.473

50 DEGREE SLOPE AT X = 11.47138
30 DEGREE SLOPE AT X = 12.90245

FOR PLOTTER

XARRAY	YARRAY	ZARRAY
10.81978	7.15600	7.15088
11.28978	7.80210	7.81632
12.54254	9.07179	9.00499
12.92391	9.32767	9.41566
13.35348	9.54286	9.51258

CLASS VALUE = 10.

.56   82   74

PLOTTING TAPE PREPARED.

PERCENT CHROMIUM IN LOW ALLOY STEEL CR 2822.4/BKGND

LN CONCENTRATION

LN INTENSITY RATIO

13 12 11 10 9 8 7 6 5 4 3 2

0 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17

0.860−
0.740−
0.540−
0.260−
0.230−
0.130−
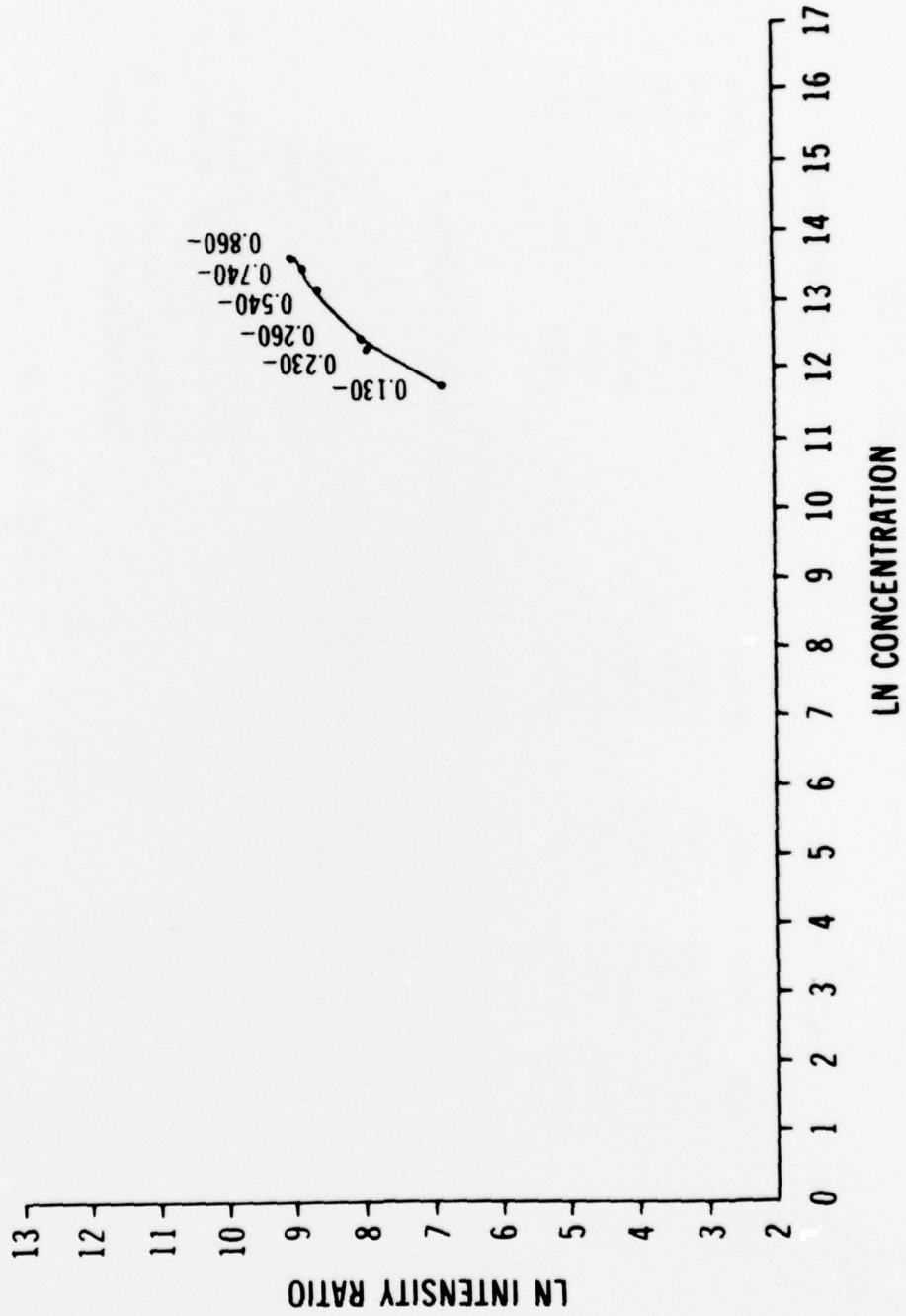
PERCENT CHROMIUM IN LOW ALLOY STEEL CR 2822.4/BKGND

NO. 2-5

TABLE OF RESIDUALS

NO. POINT	X VALUE	Y VALUE	Y ESTIMATE	RESIDUAL
1	13.66469	9.03205	8.95408	.07797
2	13.51441	8.86636	8.90531	-.03896
3	13.19932	8.64274	8.73748	-.09474
4	12.46844	8.00642	8.00617	.00025
5	12.34583	7.93337	7.83669	.09669
6	11.77529	6.82984	6.87106	-.04122

TABLE OF EXPONENTIALS

NO. POINT	X VALUE	Y VALUE	Y ESTIMATE
1	860000	8366	7739
2	740000	7089	7371
3	540000	5668	6232
4	259999	3000	2999
5	230000	2788	2531
6	130000	925	963

FORM OF EQUATION IS $Y = C + B(X) + A(X)(X)$ WHERE $Y = LN(INTENSITY)$
AND $X = LN(1,000,000$ TIMES 0 ELEMENT)

COEF. - EQUA. NO. 2   A = SECOND DEGREE TERM......-.44734893
B = FIRST DEGREE TERM......12.48302500
C = CONSTANT TERM.........-78.09191674

STD. DEV. = .09595   VERTEX (X) = 13.95222

FOR PLOTTER

XARRAY	YARRAY	ZARRAY
11.77529	6.87106	6.82984
12.34583	7.83669	7.93337
12.46844	8.00617	8.00642
13.19932	8.73748	8.64274
13.51441	8.90531	8.86636
13.66469	8.95408	9.03205

SLOPE POINT(X) = 13.61692
POINTS POINT(Y) = 6.82983

USE AN UPPER LIMIT OF 13.66469   .257
USE A LOWER LIMIT OF 11.77529   1.948

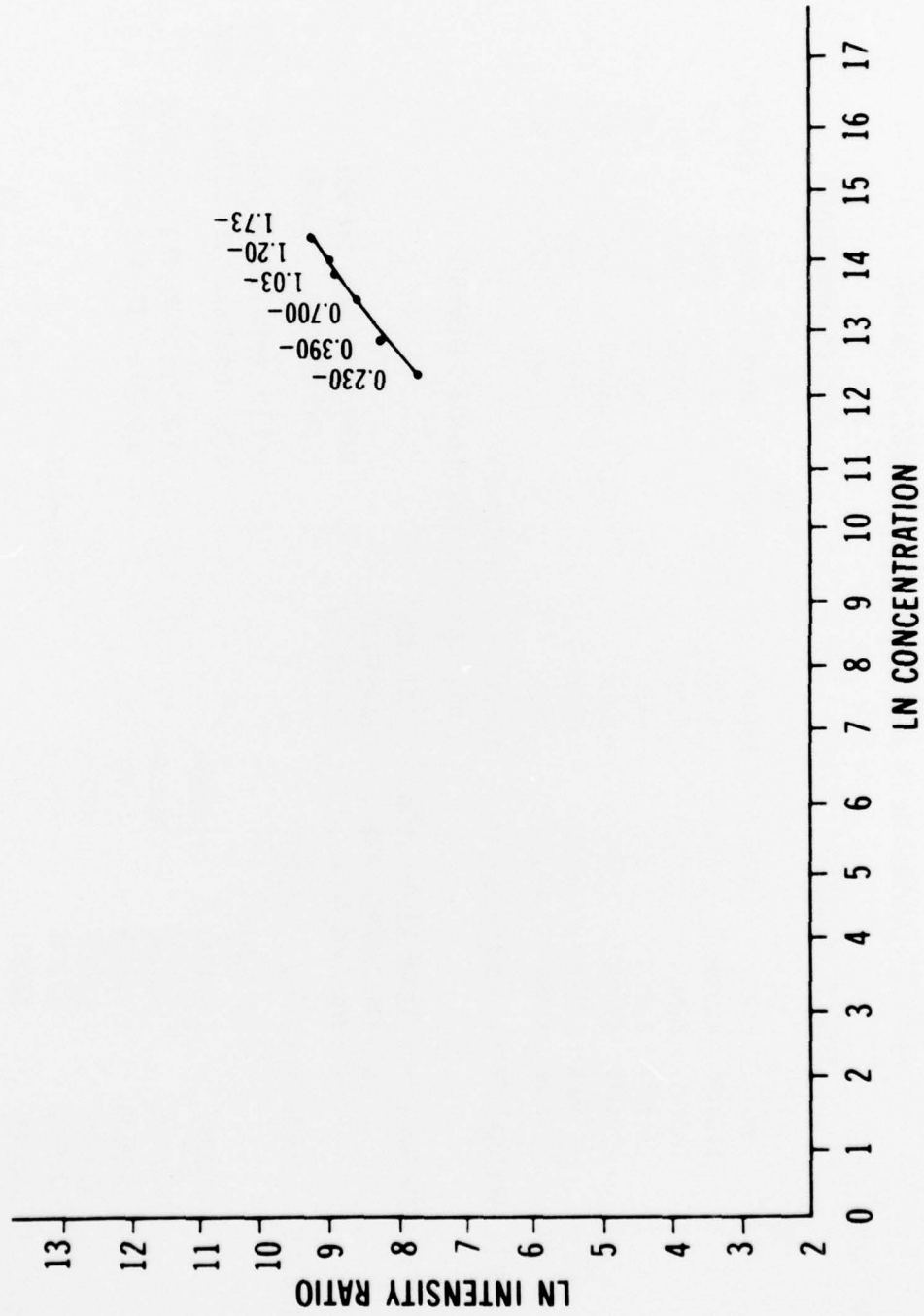50 DEGREE SLOPE AT X = 12.61099
30 DEGREE SLOPE AT X = 13.28161

CLASS VALUE = 10.

.35   79   56

PLOTTING TAPE PREPARED.

PERCENT NICKEL IN LOW ALLOY STEEL N1 3012.0/BKGND

LN CONCENTRATION

LN INTENSITY RATIO

14

PERCENT NICKEL IN LOW ALLOY STEEL N1 3012.0/BKGND

NO. 4-5

TABLE OF RESIDUALS

NO. POINT	X VALUE	Y VALUE	Y ESTIMATE	RESIDUAL
1	14.36363	9.32941	9.30745	.02196
2	13.99783	9.04396	9.06852	-.02456
3	13.84507	8.96076	8.96356	-.00289
4	13.45884	8.66031	8.68517	-.02487
5	12.87390	8.28055	8.22638	.05356
6	12.34583	7.75244	7.77564	-.02320

TABLE OF EXPONENTIALS

NO. POINT	X VALUE	Y VALUE	Y ESTIMATE
1	1730000	11264	11019
2	1200000	8467	8677
3	1030000	7791	7813
4	699999	5769	5914
5	390000	3946	3740
6	230000	2327	2381

FORM OF EQUATION IS $Y = C + B(X) + A(X)(X)$ WHERE $Y = LN(INTENSITY)$
AND $X = LN(1,000.000 \text{ TIMES } 0 \text{ ELEMENT})$

COEF. - EQUA. NO. 4 A = SECOND DEGREE TERM...... .06414837
B = FIRST DEGREE TERM....... 2.47252057
C = CONSTANT TERM......... -12.97222238

STD. DEV. = .04131   VERTEX (X) = 19.27189

SLOPE POINT(X) = 16.93356
POINTS POINT(Y) = 7.75243

USE AN UPPER LIMIT OF 14.36363   .630
USE A LOWER LIMIT OF 12.34583   .889

50 DEGREE SLOPE AT X = 9.91857
30 DEGREE SLOPE AT X = 14.59523

CLASS VALUE = 10.

100   0   0   0

FOR PLOTTER

XARRAY	YARRAY	ZARRAY
12.34583	7.77564	7.75244
12.87390	8.22698	8.28055
13.45884	8.68517	8.66031
13.84507	8.96366	8.96076
13.99783	9.06852	9.04396
14.36363	9.30745	9.32941

PLOTTING TAPE PREPARED.

DISTRIBUTION FOR MERADCOM REPORT 2110

No. Copies	Addressee	No. Copies	Addressee
	Department of Defense	2	Director, Army Materials and Mechanics Research Center ATTN: DRXMR-M (Fred Stenton) Watertown, MA 02172
12	Defense Documentation Center Cameron Station Alexandria, VA 22314		
	Department of the Army	1	US Army Aviation School Lib P.O. Drawer O Fort Rucker, AL 36360
6	Commander, US Army Materiel Development & Readiness Cmd ATTN: DRCRD-WB DRCRD-T DRCRD-J DRCRD-O DRCRD-G DRCRD-FP 5001 Eisenhower Ave Alexandria, VA 22333		**MERADCOM**
		1	DRDME-V (Material Technology Lab)
		5	DRDME-VO (Chemical Research Group)
1	Commander US Army Missile Research & Development Command ATTN: DRSMI-RR Redstone Arsenal, AL 35809	3	DRDME-JJ (Technical Reports Office)
		3	DRDME-S (Security Office)
1	Director, Army Materials and Mechanics Research Center ATTN: DRXMR-STL, Technical Library Watertown, MA 02172	2	DRDME-W (Technical Library)
		1	DRDME-I (Public Affairs Office)
		1	DRDME-BS (Arthur Nickless)